

CONGRUENCES INVOLVING MULTIPLE HARMONIC SUMS AND FINITE MULTIPLE ZETA VALUES

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ABSTRACT. Let p be a prime and \mathfrak{P}_p the set of positive integers which are prime to p . Recently, Wang and Cai proved that for every positive integer r and prime $p > 2$

$$\sum_{\substack{i+j+k=p^r \\ i,j,k \in \mathfrak{P}_p}} \frac{1}{ijk} \equiv -2p^{r-1}B_{p-3} \pmod{p^r},$$

where B_{p-3} is the $(p-3)$ -rd Bernoulli number. In this paper we prove the following analogous result: Let $n = 2$ or 4 . Then for every positive integer $r \geq n/2$ and prime $p > 4$

$$\sum_{\substack{i_1+\dots+i_n=p^r \\ i_1,\dots,i_n \in \mathfrak{P}_p}} \frac{1}{i_1 i_2 \dots i_n} \equiv -\frac{n!}{n+1} p^r B_{p-n-1} \pmod{p^{r+1}}.$$

Moreover, by using integer relation detecting tool PSLQ we can show that generalizations with larger integers n should involving finite multiple zeta values generated by Bernoulli numbers.

1. INTRODUCTION

In the study of congruence properties of multiple harmonic sums in [10, 11] the author of the current paper found the following curious congruence for every prime $p \geq 3$:

$$\sum_{\substack{i+j+k=p \\ i,j,k \geq 1}} \frac{1}{ijk} \equiv -2B_{p-3} \pmod{p}, \quad (1)$$

where B_j is the Bernoulli number defined by the generating power series

$$\frac{x}{e^x - 1} = \sum_{j=0}^{\infty} \frac{B_j}{j!} x^j.$$

A simpler proof of (1) was presented in [3]. Since then this congruence has been generalized along several directions. First, Zhou and Cai [13] showed that

$$\sum_{\substack{l_1+l_2+\dots+l_n=p \\ l_1,l_2,\dots,l_n \geq 1}} \frac{1}{l_1 l_2 \dots l_n} \equiv \begin{cases} -(n-1)!B_{p-n} & \pmod{p}, \quad \text{if } n \text{ is odd;} \\ -\frac{n \cdot n!}{2(n+1)} B_{p-n-1} p & \pmod{p^2}, \quad \text{if } n \text{ is even.} \end{cases} \quad (2)$$

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Later, Xia and Cai [9] generalized (1) to a super congruence (i.e., with higher prime powers as moduli)

$$\sum_{\substack{i+j+k=p \\ i,j,k \geq 1}} \frac{1}{ijk} \equiv -\frac{12B_{p-3}}{p-3} - \frac{3B_{2p-4}}{p-4} \pmod{p^2}$$

for every prime $p \geq 7$ while Shen and Cai [5] studied the alternating case. Let \mathfrak{P}_p be the set of positive integers which are prime to p . Recently, Wang and Cai [8] proved for every prime $p \geq 3$ and positive integer r

$$\sum_{\substack{i+j+k=p^r \\ i,j,k \in \mathfrak{P}_p}} \frac{1}{ijk} \equiv -2p^{r-1}B_{p-3} \pmod{p^r}.$$

By numerical experiment we found the following super congruences.

Theorem 1.1. *Let $n = 2$ or 4 . Then for every positive integer $r \geq n/2$ and prime $p \geq 5$ we have*

$$T_n(p, r) := \sum_{\substack{i_1 + \dots + i_n = p^r \\ i_1, \dots, i_n \in \mathfrak{P}_p}} \frac{1}{i_1 i_2 \dots i_n} \equiv -\frac{n!}{n+1} p^r B_{p-n-1} \pmod{p^{r+1}},$$

The main idea of the proof of Theorem 1.1 is to relate $T_n(p, r)$ to the p -restricted *multiple harmonic sums* (MHS for short) defined by

$$\mathcal{H}_n(s_d, \dots, s_1) := \sum_{0 < k_1 < \dots < k_d < n, \ k_1, \dots, k_d \in \mathfrak{P}_p} \frac{1}{k_1^{s_1} \dots k_d^{s_d}}, \quad (3)$$

for all positive integers n, s_1, \dots, s_d . We call d the *depth* and $s_1 + \dots + s_d$ the *weight*. One of the most important properties of the MHS is that they satisfy the so-called *shuffle relations*. For example, for all $a, b, c, n \in \mathbb{N}$ we have

$$\begin{aligned} \mathcal{H}_n(a)\mathcal{H}_n(b) &= \mathcal{H}_n(a, b) + \mathcal{H}_n(b, a) + \mathcal{H}_n(a+b), \\ \mathcal{H}_n(a, b)\mathcal{H}_n(c) &= \mathcal{H}_n(a, b, c) + \mathcal{H}_n(a, c, b) + \mathcal{H}_n(c, a, b) \\ &\quad + \mathcal{H}_n(a+c, b) + \mathcal{H}_n(a, b+c). \end{aligned} \quad (4)$$

It turns out the case $n = 2$ of Theorem 1.1 is almost trivial whereas the case $n = 4$ is much more complicated on which we will concentrate in the main body of this paper.

In the last section, we will discuss some possible generalizations using the theory of finite multiple zeta values which have been investigated in [12].

2. FIRST STEP: REDUCTION TO SUB-SUMS

We have

$$\begin{aligned} T_4(p, r) &= \frac{1}{p^r} \sum_{\substack{i_1+i_2+i_3+i_4=p^r \\ i_1, i_2, i_3, i_4 \in \mathfrak{P}_p}} \frac{i_1+i_2+i_3+i_4}{i_1 i_2 i_3 i_4} = \frac{4}{p^r} \sum_{\substack{u_3=i_1+i_2+i_3 < p^r \\ i_1, i_2, i_3, u_3 \in \mathfrak{P}_p}} \frac{i_1+i_2+i_3}{i_1 i_2 i_3} \frac{1}{u_3} \\ &= \frac{12}{p^r} \sum_{\substack{u_2=i_1+i_2 < u_3 < p^r \\ i_1, i_2, u_3, u_3-u_2 \in \mathfrak{P}_p}} \frac{i_1+i_2}{i_1 i_2} \frac{1}{u_2 u_3} = \frac{24}{p^r} \sigma(p^r), \end{aligned} \quad (5)$$

where

$$\sigma(p^r) = \sum_{\substack{0 < u_1 < u_2 < u_3 < p^r \\ u_1, u_3, u_2 - u_1, u_3 - u_2 \in \mathfrak{P}_p}} \frac{1}{u_1 u_2 u_3}.$$

Define for all positive integers a, b, c and integers $0 < i, j \leq 3$

$$\mathcal{H}_{p^r}^{i,j}(c, b, a) := \sum_{\substack{0 < u_1 < u_2 < u_3 < p^r \\ u_1, u_3 \in \mathfrak{P}_p, u_i \equiv u_j \pmod{p}}} \frac{1}{u_1^a u_2^b u_3^c}$$

and for all positive integers d, s_1, \dots, s_d

$$\mathcal{H}_{p^r}^{(d)}(s_d, \dots, s_1) := \sum_{\substack{0 < u_1 < \dots < u_d < p^r, u_1 \in \mathfrak{P}_p \\ u_1 \equiv u_2 \equiv \dots \equiv u_d \pmod{p}}} \frac{1}{u_1^{s_1} \dots u_d^{s_d}}.$$

Then by the Inclusion-Exclusion Principle

$$\sigma(p^r) = \underbrace{\mathcal{H}_{p^r}^{1,1}(1, 1, 1)}_{s_I} - \underbrace{(\mathcal{H}_{p^r}^{1,2}(1, 1, 1) + \mathcal{H}_{p^r}^{2,3}(1, 1, 1))}_{s_{II}} + \underbrace{\mathcal{H}_{p^r}^{(3)}(1, 1, 1)}_{s_{III}}. \quad (6)$$

In the next few sections we shall evaluate the three sub-sums s_I , s_{II} and s_{III} separately modulo p^{2r+1} .

3. EVALUATION OF FIRST SUB-SUM s_I IN (6)

Set

$$\mathcal{H}_{p^r}^{(2=0)}(1, 1, 1) := \sum_{\substack{0 < u_1 < u_2 < u_3 < p^r \\ u_1, u_3 \in \mathfrak{P}_p, u_2 \equiv 0 \pmod{p}}} \frac{1}{u_1 u_2 u_3}.$$

Clearly we have

$$\mathcal{H}_{p^r}^{1,1}(1, 1, 1) = \mathcal{H}_{p^r}(1, 1, 1) + \mathcal{H}_{p^r}^{(2=0)}(1, 1, 1). \quad (7)$$

Lemma 3.1. *For every prime $p \geq 5$ and positive integer $r \geq 2$ we have*

$$\mathcal{H}_{p^r}^{(2=0)}(1, 1, 1) \equiv 0 \pmod{p^{2r+1}}.$$

Proof. By the well-known formula of sums of powers (see [2, p. 230]) we have

$$P(m, n) := \sum_{j=1}^{n-1} j^m = \frac{1}{m+1} \sum_{k=0}^m \binom{m+1}{k} B_k n^{m+1-k}. \quad (8)$$

Then for all $0 < a, b, c \leq 2$ we have

$$\begin{aligned} & \mathcal{H}_{p^r}^{(2=0)}(1, 1, 1) \\ &= \frac{1}{2} \sum_{\substack{0 < u_1 < u_2 < u_3 < p^r \\ u_1, u_3 \in \mathfrak{P}_p, u_2 \equiv 0 \pmod{p}}} \left(\frac{1}{u_1 u_2 u_3} + \frac{1}{(p^r - u_1)(p^r - u_2)(p^r - u_3)} \right) \\ &\equiv -\frac{p^r}{2} \left[\mathcal{H}_{p^r}^{(2=0)}(1, 1, 2) + \mathcal{H}_{p^r}^{(2=0)}(1, 2, 1) + \mathcal{H}_{p^r}^{(2=0)}(2, 1, 1) \right] \\ &\quad - \frac{p^{2r}}{2} \left[\mathcal{H}_{p^r}^{(2=0)}(1, 1, 3) + \mathcal{H}_{p^r}^{(2=0)}(1, 3, 1) + \mathcal{H}_{p^r}^{(2=0)}(3, 1, 1) \right] \end{aligned}$$

$$+ \mathcal{H}_{p^r}^{(2=0)}(1, 2, 2) + \mathcal{H}_{p^r}^{(2=0)}(2, 2, 1) + \mathcal{H}_{p^r}^{(2=0)}(2, 1, 2) \Big] \pmod{p^{2r+1}}.$$

Now if $u_2 \equiv 0 \pmod{p}$ then we write $u_2 = vp^\beta$ where $v \in \mathfrak{P}_p$. Then

$$\begin{aligned} \mathcal{H}_{p^r}^{(2=0)}(c, b, a) &= \sum_{\beta=1}^{r-1} \sum_{\substack{1 \leq v < p^{r-\beta} \\ v \in \mathfrak{P}_p}} \left(\sum_{\substack{0 < u_1 < vp^\beta < u_3 < p^r \\ u_1, u_3 \in \mathfrak{P}_p}} \frac{1}{u_1^a (vp^\beta)^b u_3^c} \right) \\ &= \sum_{\beta=1}^{r-1} \sum_{\substack{1 \leq v < p^{r-\beta} \\ v \in \mathfrak{P}_p}} \frac{1}{v^b p^{\beta b}} \left(\sum_{0 < u_1 < vp^\beta, u_1 \in \mathfrak{P}_p} \frac{1}{u_1^a} \right) \left(\sum_{vp^\beta < u_3 < p^r, u_3 \in \mathfrak{P}_p} \frac{1}{u_3^c} \right). \end{aligned}$$

Let $m = \varphi(p^{2r+1})$. Then $m > 4$ for every prime $p \geq 5$. Thus

$$\sum_{0 < u < vp^\beta, u \in \mathfrak{P}_p} \frac{1}{u^a} \equiv \sum_{u=1}^{vp^\beta-1} u^{m-a} \equiv vp^\beta B_{m-a} + p^{2\beta} f(v) \pmod{p^{r+1+\beta}}$$

where $f(x) \in x\mathbb{Z}_p[x]$ is some polynomial with p -integral coefficients. Further

$$\begin{aligned} \sum_{vp^\beta < u < p^r, u \in \mathfrak{P}_p} \frac{1}{u^c} &\equiv \sum_{u=1}^{p^r-1} u^{m-c} - \sum_{u=1}^{vp^\beta-1} u^{m-c} \\ &\equiv (p^r - vp^\beta) B_{m-c} + p^{2\beta} g(v) \pmod{p^{r+1+\beta}} \end{aligned}$$

where $g(x) \in x\mathbb{Z}_p[x]$ is a polynomial with p -integral coefficients. Now we divide (a, b, c) into two cases: (i) $a + b + c = 4$ and (ii) $a + b + c = 5$.

In case (i) we see that $B_{m-c} B_{m-a} = 0$ since m is even and one of a or c is 1. Hence

$$\begin{aligned} \mathcal{H}_{p^r}(c, b, a) &\equiv \sum_{\beta=1}^{r-1} \sum_{\substack{1 \leq v < p^{r-\beta} \\ v \in \mathfrak{P}_p}} v^{m-b} \left[p^{r+(2-b)\beta} B_{m-c} f(v) - vp^{(3-b)\beta} B_{m-c} f(v) \right. \\ &\quad \left. + vp^{(3-b)\beta} B_{m-a} g(v) + p^{(4-b)\beta} g(v) f(v) \right] \pmod{p^{r+1}}. \end{aligned}$$

Note that m is even so $B_{m-c} \neq 0$ if and only if $(a, b, c) = (1, 1, 2)$. Similar arguments for the four terms in the above shows that $\mathcal{H}_{p^r}(c, b, a) \equiv 0 \pmod{p^{r+1}}$ since $1 \leq \beta \leq r-1$ and for all $i \geq 1$

$$\sum_{v=1}^{p^{r-\beta}-1} v^i \equiv 0 \pmod{p^{r-\beta}}.$$

In case (ii) we only need to show $\mathcal{H}_{p^r}(c, b, a) \equiv 0 \pmod{p}$ which is much easier than the case (i) so we leave it to the interested reader. \square

Lemma 3.2. *For every prime $p \geq 5$ and positive integer $r \geq 2$ we have*

$$\mathcal{H}_{p^r}^{1,1}(1, 1, 1) \equiv \mathcal{H}_{p^r}(1, 1, 1) \equiv -\frac{2}{5} B_{p-5} p^{2r} \pmod{p^{2r+1}}. \quad (9)$$

Proof. Let $m = \varphi(p^{2r+1}) - 1$. Then $m \geq 2r + 1$ for every prime $p \geq 5$. Thus

$$\mathcal{H}_{p^r}(1, 1, 1) \equiv \sum_{0 < u_1 < u_2 < u_3 < p^r} u_1^m u_2^m u_3^m \equiv H_{p^r}(m, m, m)$$

$$\equiv \frac{1}{6} \left[H_{p^r}(m)^3 - 3H_{p^r}(2m)H_{p^r}(m) + 2H_{p^r}(3m) \right] \pmod{p^{2r+1}}$$

by the stuffle relations (4). Noticing that m is odd, by (8) we get

$$H_{p^r}(m) \equiv 0 \pmod{p^{r+1}} \quad \text{and} \quad H_{p^r}(2m) \equiv 0 \pmod{p^r}.$$

Hence by (8) we get

$$\mathcal{H}_{p^r}(1, 1, 1) \equiv \frac{1}{3} H_{p^r}(3m) \equiv \frac{m}{2} p^{2r} B_{3m-1} \equiv -\frac{1}{2} p^{2r} B_{3m-1} \pmod{p^{2r+1}}.$$

Now the lemma follows immediately from the following Kummer congruence

$$\frac{B_{3m-1}}{3m-1} \equiv \frac{B_{p-5}}{p-5} \pmod{p} \quad (10)$$

and Lemma 3.1. □

4. EVALUATION OF THE THIRD SUB-SUMS s_{III} IN (6)

In this section we will use stuffle relations to evaluate the sub-sum s_{III} of (6) modulo p^{2r+1} . Some parts of the following lemma are similar to (or generalizations) of [8, Lemma 3]. For completeness we provide the details of its proof.

Lemma 4.1. *Let x be an integer in such that $0 < x < p$. For all positive integers r , k , and prime $p \geq 3$ we set*

$$S_k(x, p^r) = \sum_{0 < i < p^r, i \equiv x \pmod{p}} \frac{1}{i^k}.$$

Then we have

- (i) $S_k(x, p^2) \equiv p S_k(x, p) \pmod{p^2}$ and $S_k(x, p^{r+1}) \equiv p S_k(x, p^r) \pmod{p^{r+2}}$ for $r \geq 2$ and $k \geq 1$. Moreover, for any integer $\ell \geq 0$ and $r \geq 2$ we have

$$\sum_{x=1}^{p-1} x^\ell (S_k(x, p^{r+1}) - p S_k(x, p^r)) \equiv 0 \pmod{p^{r+3}}. \quad (11)$$

- (ii) $S_k(x, p^r) \equiv 0 \pmod{p^{r-1}}$ for $r \geq 2$.
 (iii) $\{S_k(x, p^{r+1})\}^d \equiv p^d \{S_k(x, p^r)\}^d \pmod{p^{dr+2}}$ for $r \geq 2$ and $d \geq 1$.
 (iv) $\{S_k(x, p^r)\}^d \equiv p^{d(r-1)} x^{-dk} + \frac{dk}{2} p^{d(r-1)+1} x^{-dk-1} \pmod{p^{d(r-1)+2}}$ for all $d \geq 1$ and $r \geq 2$.
 (v) Let $r \geq 2$ and $d, k \in \mathbb{N}$ such that $dk < p-1$. Then we have

$$\sum_{x=1}^{p-1} \{S_k(x, p^r)\}^d \equiv \frac{dk p^{d(r-1)+1}}{dk+1} B_{p-1-dk} \pmod{p^{d(r-1)+2}}.$$

- (vi) $S_1(x, p^{r+1}) S_2(x, p^{r+1}) \equiv p^2 S_1(x, p^r) S_2(x, p^r) \pmod{p^{2r+2}}$ for $r \geq 2$. Moreover, for every integer $r \geq 2$ we have

$$\sum_{x=1}^{p-1} S_1(x, p^r) S_2(x, p^r) \equiv 0 \pmod{p^{2r+1}}. \quad (12)$$

Proof. (i) By definition, if $r = 1$ we have

$$S_k(x, p^2) - pS_k(x, p) = \sum_{0 < j < p} \frac{1}{(x + jp)^k} - \frac{p}{x^k} \equiv - \sum_{0 < j < p} \frac{kjp}{x^k} \equiv 0 \pmod{p^2}.$$

If $r \geq 2$ then

$$\begin{aligned} & S_k(x, p^{r+1}) - pS_k(x, p^r) \\ &= \sum_{0 < j < p^r} \frac{1}{(x + jp)^k} - p \sum_{0 \leq a < p^{r-1}} \frac{1}{(x + ap)^k} \\ &= \sum_{b=1}^{p-1} \left(\sum_{0 \leq a < p^{r-1}} \frac{1}{(x + (a + p^{r-1}b)p)^k} - \frac{1}{(x + ap)^k} \right) \\ &= -p^r \sum_{b=1}^{p-1} b \sum_{0 \leq a < p^{r-1}} \frac{\sum_{l=0}^{k-1} (x + ap)^l (x + (a + p^{r-1}b)p)^{k-1-l}}{(x + (a + p^{r-1}b)p)^k (x + ap)^k} \\ &\equiv -p^r \sum_{b=1}^{p-1} b \sum_{0 \leq a < p^{r-1}} \frac{k(x + ap)^{k-1}}{(x + ap)^{2k}} \equiv 0 \pmod{p^{r+2}} \end{aligned}$$

since $p^r \equiv 0 \pmod{p^2}$, $\sum_{b=1}^{p-1} b \equiv 0 \pmod{p}$ and

$$\sum_{0 \leq a < p^{r-1}} \frac{k(x + ap)^{k-1}}{(x + ap)^{2k}} \equiv \sum_{0 \leq a < p^{r-1}} \frac{k}{x^{k+1}} \equiv \frac{kp^{r-1}}{x^{k+1}} \equiv 0 \pmod{p}.$$

Further, for any integer $\ell \geq 0$ and $r \geq 2$ we have modulo p^{r+3}

$$\sum_{x=1}^{p-1} x^\ell (S_k(x, p^{r+1}) - pS_k(x, p^r)) \equiv -p^r \sum_{x=1}^{p-1} \sum_{b=1}^{p-1} b \sum_{0 \leq a < p^{r-1}} \frac{kx^\ell}{(x + ap)^{k+1}} \equiv 0$$

since now for $m = \varphi(p^2) - k - 1$ we have

$$\sum_{x=1}^{p-1} \sum_{0 \leq a < p^{r-1}} \frac{x^\ell}{(x + ap)^{k+1}} \equiv \sum_{x=1}^{p-1} \sum_{0 \leq a < p^{r-1}} x^\ell (x + ap)^m \pmod{p^2}$$

and for any integer $\alpha, \beta \geq 0$ we have

$$\sum_{x=1}^{p-1} x^\alpha \equiv \sum_{0 \leq a < p^{r-1}} a^\beta \equiv 0 \pmod{p}.$$

(ii) This follows from (i) by an easy induction on r .

(iii) This follows from (i) and (ii) by the formula

$$A^d - B^d = (A - B) \sum_{j=0}^{d-1} A^j B^{j-d}.$$

(iv) If $r = 2$ then let $m = \varphi(p^{d+2}) - k$. We get

$$S_k(x, p^2) = \sum_{j=0}^{p-1} \frac{1}{(x + jp)^k} \equiv \sum_{j=0}^{p-1} (x + jp)^m \pmod{p^{d+2}}.$$

Expanding and noticing that $m \equiv -k \pmod{p}$, we get

$$S_k(x, p^2) \equiv px^m + \frac{k}{2}p^2x^{m-1} + p^3f(x) \pmod{p^{d+2}}$$

for some polynomial $f(x) \in x\mathbb{Z}_p[x]$. Thus

$$\{S_k(x, p^2)\}^d \equiv p^d x^{dm} + \frac{dk}{2}p^{d+1}x^{dm-1} \pmod{p^{d+2}}.$$

Now (iv) follows from induction on r by using (iii).

(v) This follows from (iv) immediately.

(vi) Set $m = \varphi(p^5) - 2$. By (iv) there are polynomials $f(x), g(x), h(x) \in x\mathbb{Z}_p[x]$ such that

$$\begin{aligned} & \sum_{x=1}^{p-1} S_1(x, p^2) S_2(x, p^2) \\ & \equiv \sum_{x=1}^{p-1} \left[px^{m+1} + \frac{1}{2}p^2x^m + p^3f(x) \right] \left[px^m + p^2x^{m-1} + p^3g(x) \right] \\ & \equiv \sum_{x=1}^{p-1} \left[p^2x^{2m+1} + \frac{3}{2}p^3x^{2m} + p^4h(x) \right] \\ & \equiv \frac{2m+1}{2}p^4B_{2m} + \frac{3}{2}p^4B_{2m} \equiv 0 \pmod{p^5} \end{aligned} \tag{13}$$

since $2m+1 \equiv -3 \pmod{p}$. This proves (vi) for $r = 2$.

For the general case, similar to (iii) we have

$$\begin{aligned} & S_1(x, p^{r+1}) S_2(x, p^{r+1}) - p^2 S_1(x, p^r) S_2(x, p^r) \\ & = S_2(x, p^{r+1}) [S_1(x, p^{r+1}) - p S_1(x, p^r)] + p S_1(x, p^r) [S_2(x, p^{r+1}) - p S_2(x, p^r)] \\ & \equiv 0 \pmod{p^{2r+2}} \end{aligned}$$

by (i) and (ii). Moreover, for each x there exist $f(x), g(x) \in \mathbb{Z}_p[x]$ such that

$$S_2(x, p^{r+1}) = p^r f(x), \quad \text{and} \quad p S_1(x, p^r) = p^r g(x).$$

Thus from (11) and by induction on r we can show that

$$\begin{aligned} \sum_{x=1}^{p-1} S_1(x, p^r) S_2(x, p^r) & \equiv p^2 \sum_{x=1}^{p-1} S_1(x, p^{r-1}) S_2(x, p^{r-1}) \\ & \equiv \cdots \equiv p^{2r-4} \sum_{x=1}^{p-1} S_1(x, p^2) S_2(x, p^2) \equiv 0 \pmod{p^{2r+1}} \end{aligned}$$

because of (13). □

We can now consider the second sub-sums of (6) modulo p^{2r+1}

Lemma 4.2. *For every prime $p \geq 5$ and positive integer $r \geq 2$ we have*

$$\begin{aligned}\mathcal{H}_{p^r}^{(2)}(1, 2) + \mathcal{H}_{p^r}^{(2)}(2, 1) &\equiv \frac{6}{5}B_{p-5}p^{2r} \pmod{p^{2r+1}}, \\ \mathcal{H}_{p^r}(3) &\equiv -\frac{6}{5}B_{p-5}p^{2r} \pmod{p^{2r+1}}.\end{aligned}\tag{14}$$

Proof. It is easy to see that

$$\mathcal{H}_{p^r}^{(2)}(1, 2) + \mathcal{H}_{p^r}^{(2)}(2, 1) + \mathcal{H}_{p^r}(3) \equiv \sum_{x=1}^{p-1} S_1(x, p^r) S_2(x, p^r) \equiv 0 \pmod{p^{2r+1}}$$

by (12). Setting $m = \varphi(p^{2r+1}) - 3$ and noticing m is odd we get

$$\mathcal{H}_{p^r}(3) \equiv \sum_{u=1}^{p^r-1} u^m \equiv \frac{m}{2}p^{2r}B_{m-1} \equiv -\frac{3}{2}p^{2r}B_{m-1} \equiv -\frac{6}{5}p^{2r}B_{p-5} \pmod{p^{2r+1}}$$

by the Kummer congruence

$$\frac{B_{m-1}}{m-1} \equiv \frac{B_{p-5}}{p-5} \pmod{p}.$$

The lemma now follows at once. \square

Finally we deal with the sub-sum s_{III} of (6) modulo p^{2r+1} .

Corollary 4.3. *For every prime $p \geq 5$ and positive integer $r \geq 2$ we have*

$$\mathcal{H}_{p^r}^{(3)}(1, 1, 1) \equiv -\frac{2}{5}B_{p-5}p^{2r} \pmod{p^{2r+1}}.\tag{15}$$

Proof. By stuffle relation (4) we have

$$6\mathcal{H}_{p^r}^{(3)}(1, 1, 1) + 3(\mathcal{H}_{p^r}^{(2)}(1, 2) + \mathcal{H}_{p^r}^{(2)}(2, 1)) + \mathcal{H}_{p^r}(3) = \sum_{x=1}^{p-1} \{S_1(x, p^r)\}^3 \equiv 0 \pmod{p^{2r+1}}$$

by Lemma 4.1(v). So the corollary follows quickly from Lemma 4.2. \square

5. EVALUATION OF THE SECOND SUB-SUMS s_{II} IN (6)

It turns out s_{II} is the most difficult to evaluate modulo p^{2r+1} . We will use repeatedly (and often implicitly) the fact that

$$\sum_{w=1}^{p^s-1} w^\ell \equiv \begin{cases} 0 & \pmod{p^s}, & \text{if } \ell \text{ is even;} \\ 0 & \pmod{p^{s+1}}, & \text{if } \ell \text{ is odd.} \end{cases}\tag{16}$$

Lemma 5.1. *For every positive integer $r \geq 2$ and prime $p \geq 5$ we have*

$$\mathcal{H}_{p^r}^{1,3}(1, 1, 1) \equiv -\frac{3}{5}p^{2r}B_{p-5} \pmod{p^{2r+1}}.\tag{17}$$

Proof. Let $m = \varphi(p^{2r+1}) - 1$. Modulo p^{2r+1} we have

$$\mathcal{H}_{p^r}^{1,3}(1, 1, 1) \equiv \sum_{v=1}^{p^{r-1}-1} \sum_{0 < u < u_1 < u+vp < p^r} u^m u_1^m (u+vp)^m$$

$$\begin{aligned}
&\equiv \sum_{v=1}^{p^{r-1}-1} \sum_{0 < u < p^r - vp} [P(m, u + vp) - u^m - P(m, u)](u + vp)^m u^m, \\
&\equiv \sum_{v=1}^{p^{r-1}-1} \sum_{0 < u < vp} [P(m, u + p^r - vp) - u^m - P(m, u)](u + p^r - vp)^m u^m,
\end{aligned}$$

by changing the index $v \rightarrow p^{r-1} - v$. Observe

$$\begin{aligned}
P(m, u + p^r - vp) &= \sum_{k=0}^m \frac{\binom{m+1}{k}}{m+1} (u + p^r - vp)^{m+1-k} B_k \\
&\equiv \sum_{k=0}^m \frac{\binom{m+1}{k}}{m+1} [(u - vp)^{m+1-k} + (m+1-k)p^r(u - vp)^{m-k}] B_k \\
&\equiv \sum_{k=0}^m \frac{\binom{m+1}{k}}{m+1} (vp - u)^{m+1-k} B_k + (vp - u)^m + p^r F(u - vp) - \frac{m}{2} p^r (u - vp)^{m-1} \\
&\equiv P(m, vp - u) + (vp - u)^m + p^r F(u - vp) + \frac{1}{2} p^r (u - vp)^{m-1} \pmod{p^{r+1}}
\end{aligned}$$

since $B_1 = -1/2$ and $B_k = 0$ for all odd $k > 2$. Here $F(x) \in x\mathbb{Z}_p[x]$ is an odd polynomial in x (i.e., only odd powers of x can appear). It is straight-forward to see that

$$\sum_{v=1}^{p^{r-1}-1} \sum_{0 < u < vp} F(u - vp)(u + p^r - vp)^m u^m \equiv 0 \pmod{p^{r+1}}.$$

Hence modulo p^{2r+1} we have

$$\begin{aligned}
\mathcal{H}_{p^r}^{1,3}(1, 1, 1) &\equiv \sum_{v=1}^{p^{r-1}-1} \sum_{0 < u < vp} [P(m, vp - u) + (vp - u)^m \\
&\quad + \frac{1}{2} p^r (u - vp)^{m-1} - u^m - P(m, u)](u + p^r - vp)^m u^m, \\
&\equiv G(p, r) + \sum_{v=1}^{p^{r-1}-1} \sum_{0 < u < vp} \left\{ \frac{1}{2} p^r (u - vp)^{m-1} (u + p^r - vp)^m u^m \right. \\
&\quad \left. + mp^r [P(m, vp - u) + (vp - u)^m - u^m - P(m, u)](u - vp)^{m-1} u^m \right\} \\
&\equiv G(p, r) + p^r \sum_{v=1}^{p^{r-1}-1} \sum_{0 < u < vp} \left\{ \frac{5}{2} u^{3m-1} + [P(m, u) - P(m, vp - u)] u^{2m-1} \right\},
\end{aligned}$$

where

$$G(p, r) = \sum_{v=1}^{p^{r-1}-1} \sum_{0 < u < vp} [P(m, vp - u) + (vp - u)^m - u^m - P(m, u)](u - vp)^m u^m.$$

By change of index $u \rightarrow vp - u$ we see clearly that $G(p, r) \equiv 0 \pmod{p^{2r+1}}$ since m is odd. Expanding $P(m, vp - u)$ and $P(m, u)$ using (8) and (16) we get

$$\begin{aligned} \mathcal{H}_{p^r}^{1,3}(1, 1, 1) &\equiv p^r \sum_{v=1}^{p^{r-1}-1} \sum_{0 < u < vp} \left\{ \frac{5}{2} u^{3m-1} + [u^m B_1 - (vp - u)^m B_1] u^{2m-1} \right\} \\ &\equiv \frac{3}{2} p^r \sum_{v=1}^{p^{r-1}-1} \sum_{0 < u < vp} u^{3m-1} \equiv \frac{3}{2} p^{r+1} \sum_{v=1}^{p^{r-1}-1} v B_{3m-1} \equiv -\frac{3}{4} p^{2r} B_{3m-1}. \end{aligned}$$

Now the lemma follows readily from by Kummer congruence

$$\frac{B_{3m-1}}{3m-1} \equiv \frac{B_{p-5}}{p-5} \pmod{p}. \quad \square$$

Lemma 5.2. *For every positive integer $r \geq 2$ and prime $p \geq 5$ we have*

$$\mathcal{H}_{p^r}^{1,2}(1, 1, 1) + \mathcal{H}_{p^r}^{2,3}(1, 1, 1) \equiv -\frac{3}{5} p^{2r} B_{p-5} \pmod{p^{2r+1}}. \quad (18)$$

Proof. By stuffle relations (4) and Lemma 4.1 we have modulo p^{2r+1} (suppressing the subscript p^r)

$$\begin{aligned} 0 &\equiv \mathcal{H}(1) \sum_{x=1}^{p-1} \{S_1(x, p^r)\}^2 = \mathcal{H}(1) [\mathcal{H}(2) + 2\mathcal{H}^{(2)}(1, 1)] = \mathcal{H}(1)\mathcal{H}(2) \\ &\quad + 2[\mathcal{H}^{1,2}(1, 1, 1) + \mathcal{H}^{2,3}(1, 1, 1) + \mathcal{H}^{1,3}(1, 1, 1)] + 2[\mathcal{H}^{(2)}(1, 2) + \mathcal{H}^{(2)}(2, 1)]. \end{aligned}$$

Since $\mathcal{H}(1)\mathcal{H}(2) \equiv 0 \pmod{p^{2r+1}}$ we can derive (18) from (14) and (17) easily. \square

6. PROOF OF THEOREM 1.1

Let $m = \varphi(p^{2r+1}) - 1$. When $n = 2$ and $r \geq 1$ we have

$$\sum_{\substack{i+j=p^r \\ i, j \in \mathfrak{P}_p}} \frac{1}{ij} = \frac{1}{p^r} \sum_{\substack{i+j=p^r \\ i, j \in \mathfrak{P}_p}} \frac{i+j}{ij} = \frac{2}{p^r} \sum_{\substack{0 < i < p^r \\ i \in \mathfrak{P}_p}} \frac{1}{i}.$$

Observing that m is odd we have

$$\sum_{\substack{0 < i < p^r \\ i \in \mathfrak{P}_p}} \frac{1}{i} \equiv \sum_{i=1}^{p^{r-1}-1} i^m \equiv \frac{m}{2} p^{2r} B_{m-1} \equiv -\frac{1}{3} p^{2r} B_{p-3} \pmod{p^{2r+1}}$$

by Kummer congruence

$$\frac{B_{m-1}}{m-1} \equiv \frac{B_{p-3}}{p-3} \pmod{p}.$$

This completes the proof of the theorem when $n = 2$.

For the case of $n = 4$ we can use (9), (15), and (18) evaluate (6) and get

$$\sigma(p^r) \equiv -\frac{1}{5} p^{2r} B_{p-5} \pmod{p^{2r+1}}.$$

So the theorem follows immediately from (5).

7. GENERALIZATIONS AND FINITE MULTIPLE ZETA VALUES

It is natural to ask if one can generalize Theorem 1.1 to the case of $n \geq 6$. By using integer relation detecting tool PSLQ (the partial sum of least squares algorithm) developed originally by Ferguson and Bailey [1] we can show that if similar congruence holds for $n = 6$, say

$$\sum_{\substack{i_1+\dots+i_6=p^2 \\ i_1,\dots,i_6 \in \mathfrak{P}_p}} \frac{1}{i_1 i_2 i_3 i_4 i_5 i_6} \equiv c_6 p^2 B_{p-7} \pmod{p^3} \quad (19)$$

for some $c_6 \in \mathbb{Q}$ and for all prime $p \geq 7$, then both the numerator and the denominator of c_6 must have at least 60 digits.

At first glance, it may seem impossible to use PSLQ to work with congruences. However, we may use the following idea, say, in case $n = 6$. Let S be the set of the first 1000 primes greater than 6. Let P be the product of these primes. By the Chinese Remainder Theorem we can find two integers A and B , between 0 and P^3 so that

$$A \equiv \sum_{\substack{i_1+\dots+i_6=p^2 \\ i_1,\dots,i_6 \in \mathfrak{P}_p}} \frac{1}{i_1 i_2 i_3 i_4 i_5 i_6}, \quad B \equiv p^2 B_{p-7} \pmod{p^3}$$

for each prime in S . If (19) were true for some $c_6 = a/b$ in reduced form with a and b both of reasonable sizes, then we would have

$$A - \frac{a}{b} B = NP^3$$

for some integer N . Thus we can use PSLQ to discover a and b .

For any positive integers $n > m \geq 1$ and prime $p > n$, define

$$R_n^{(m)}(p) := \sum_{\substack{i_1+\dots+i_n=mp \\ i_1,\dots,i_n \in \mathfrak{P}_p}} \frac{1}{i_1 \cdots i_n} \pmod{p} \in \mathbb{Z}/p\mathbb{Z}.$$

Let \mathcal{P} be the set of rational primes. It turns out that the quantity

$$\left(R_n^{(m)}(p) \right)_{p \in \mathcal{P}} \in \mathcal{A} := \prod_{p \in \mathcal{P}} (\mathbb{Z}/p\mathbb{Z}) \bigg/ \bigoplus_{p \in \mathcal{P}} (\mathbb{Z}/p\mathbb{Z}) \quad (20)$$

involves the finite multiple zeta values (FMZVs) defined as follows (see [12] for more details). For all positive integers s_1, \dots, s_d , set

$$\zeta_{\mathcal{A}}(s_1, \dots, s_d) := \left(\mathcal{H}_p(s_d, \dots, s_1) \right)_{p \in \mathcal{P}} \in \mathcal{A}.$$

The number d is called the depth and $s_1 + \dots + s_d$ the weight. Clearly, \mathbb{Q} can be embedded into \mathcal{A} diagonally. For any positive integer w , let \mathbf{FMZV}_w be the \mathbb{Q} -vector subspace generated by all the FMZVs of weight w . By the FMZV dimension conjecture discovered by Zagier and independently by the author (see [12]), we have the following data in Table 1. By [11,

w	0	1	2	3	4	5	6	7	8	9	10	11	12
$\dim \mathbf{FMZV}_w$	1	0	0	1	0	1	1	1	2	2	3	4	5

TABLE 1. Numerically verified conjectural dimensions and \mathbf{FMZV}_w .

Theorem 1.7], we see that the \mathcal{A} -Bernoulli number

$$\beta_w := \left(B_{p-w}/w \right)_{p>w+2} = \zeta_{\mathcal{A}}(w-1, 1)/w \in \text{FMZV}_w.$$

Here, we put 0 at all the components with $p < w + 1$. By stuffle relation, we obtain

$$\prod_{j=1}^n \beta_{w_j} \in \text{FMZV}_{w_1+\dots+w_n}.$$

Let BN_w be the subspace generated by all such products of \mathcal{A} -Bernoulli numbers of total weight w . From overwhelming evidence we make the following conjecture.

Conjecture 7.1. *For all positive integers $n, m \geq 1$, we have*

$$\left(R_n^{(m)}(p) \right)_{p \in \mathcal{P}} \in \text{BN}_n.$$

This conjecture is supported by (2) and the results in previous works [4, 6, 7, 10] when $n \leq 10$. By the same argument as in [6], it should be straight-forward to prove the following results: For all positive integers n, m and primes $p > 5$, we have

$$\begin{aligned} R_4^{(m)}(p) &\equiv -\frac{4!}{5}m(m^2+1)B_{p-5} \cdot p \pmod{p^2}, \\ R_8^{(m)}(p) &\equiv \frac{112}{5}m(m^2+16)(m^2-1)B_{p-3}B_{p-5} \pmod{p}. \end{aligned}$$

The corresponding result of $R_6^{(m)}(p)$ is proved by Wang in [6].

We conclude the paper by the following conjecture which has been discovered numerically by Maple computation using the PSLQ algorithm.

Conjecture 7.2. *For any positive integer m and all primes $p > 11$, we have*

$$\begin{aligned} R_{11}^{(m)}(p) &\equiv 88 \cdot 5! \binom{m+2}{5} (m^2+33) B_{p-3}^2 B_{p-5} \\ &\quad + 10m(m^8+330m^6+16401m^4+152900m^2+193248) B_{p-11} \pmod{p}, \\ R_{12}^{(m)}(p) &\equiv -\frac{55 \cdot 8!}{9} \binom{m+3}{7} B_{p-3}^4 \\ &\quad - \frac{22 \cdot 5!}{9} \binom{m+1}{3} (m^6+211m^4+6196m^2+32256) B_{p-3} B_{p-9} \\ &\quad - \frac{66 \cdot 4!}{7} \binom{m+1}{3} (m^6+187m^4+6508m^2+31392) B_{p-5} B_{p-7} \pmod{p}. \end{aligned}$$

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